Assessing Multizone Airflow Simulation Software

David M. Lorenzetti
Indoor Environment Department
Lawrence Berkeley National Laboratory, Berkeley CA 94720
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Abstract

Several standard multizone modeling programs, in order to improve their computational efficiency, make a number of simplifying assumptions. This paper examines how those assumptions reduce the solution times and memory use of the programs, but at the cost of restricting the models they can express. Applications where these restrictions may adversely affect the program's usefulness include: (1) natural ventilation, when buoyancy effects dominate mechanically-driven flow; (2) duct system design, when losses in T-junctions affect the system performance; and (3) control system design, when the dynamic transport of pollutants plays a significant role in the simulated system.

Keywords: Comis, Contam, Modeling, Multizone, Pollutant transport.

Introduction

Multizone models form the basis of most computer simulations of airflow and pollutant transport in buildings. Whole-building analysis relies on these lumped-parameter models, rather than on fluid-dynamic models, due to the high demand the latter techniques make on computer memory, processing power, and input data.

The design of the current generation of multizone programs results from a systematic drive to improve their computational efficiency, mainly by the introduction of specialized algorithms and data structures. This specialization has allowed engineers and scientists to explore a wide range of building airflow problems. However, with increased understanding of these problems has come the desire to explore questions that lie beyond the capabilities of current multizone tools.

This paper considers two popular and well-characterized multizone simulation programs, Contam (Walton, 1997) and Comis (Feustel, 1999). The paper examines how design decisions made to improve their efficiency also restrict their ability to incorporate a number of interesting, and potentially important, airflow and pollutant transport models. After describing the computational approach taken by the programs, this paper describes some new models that would be difficult to implement under the current software architecture. These models would prove useful in a number of application areas, including the study of natural ventilation and the design of novel mechanical ventilation systems.

The decision to focus on Contam and Comis follows from their popularity, and the author's familiarity with them, rather than an assessment that they are either more or less capable than other multizone programs. Furthermore, the comments made here pertain to the extremes of these programs' capabilities, and do not imply that the codes perform poorly when applied to their intended use.

Computational Approach

Multizone models idealize a building as a collection of well-mixed spaces, or zones, connected by discrete flow paths. In Contam and Comis, the user constructs a building description by assembling various component models, each representing a zone or a flow path. A simulation predicts the system's behavior based on the interactions of the assembled components. Flow path models range from simple cracks, to windows and doors, to active elements such as fans. By contrast, the programs provide only one zone model, which represents a well-mixed space with simple hydrostatic pressure variations.

Both CONTAM and COMIS decouple the airflow problem from the thermal problem (finding the temperatures in the zones) by assuming the temperatures remain fixed, for example at user-supplied values. This yields a steady-state airflow system, which can be embedded in a dynamic thermal system by treating the resulting airflows as constant until the next simulated time, when new zone temperatures produce a new steady-state airflow solution.

Similarly, the programs decouple the airflow and pollutant transport problems, by assuming the amount of pollutant in a space does not affect the airflows. Hence they idealize a building as composed of: (1) a steady-state airflow network, defined by algebraic equations which, given the zone temperatures, describe the mass conservation of air; and (2) a dynamic pollutant transport model, defined by ordinary differential equations which, given the airflows, describe the mass conservation of pollutants.

This paper mainly concerns design features in the software that solves the airflow equations. Both programs represent the state of the airflow system using the pressures in the zones. Each zone has a single reference pressure, chosen by the airflow solver. The computation proceeds by: (1) finding the pressures at the points where the flow elements connect to each zone, based on the zone reference pressures and temperatures; (2) finding the flows in each path, based on the pressures and densities of air at its terminals; and (3) summing the flows in and out of each zone. The solver adjusts the reference pressures to achieve mass balance, in other words, so that the mass flow rate of air into each zone matches the flow rate out of the zone. The program then passes these flows to the pollutant transport solver.

Modeling Restrictions

This section describes some design decisions taken in CONTAM and COMIS in order to improve the efficiency of solving the steady-state airflow network. A more complete analysis, given by Lorenzetti (2002), details the computational advantages gained by each decision. These include improved calculation speed, reduced computer memory requirements, and convergence guarantees. It is important to bear in mind that many of these decisions were made to bring multizone simulation to desktop computers with less capacity than those of today.

Probably the most important decision was to restrict the component models in a way that produces symmetric Jacobian matrices (Lorenzetti, 2002). The Jacobian stores the derivatives of the nonlinear equations that define the airflow network. At each time step, CONTAM and COMIS repeatedly calculate and factor new Jacobian matrices, extracting trial solutions for the airflow system using variations on Newton–Raphson's method. A symmetric matrix requires only about half the storage, and may be factored in about half the time, as a general full matrix (Dennis and Schnabel, 1996). In fact, the specialized sparse matrix techniques in CONTAM and COMIS run even faster than this (Walton, 1997). These efficiency gains are important since matrix factorization dominates the solution time for the nonlinear system.

In practical terms, a symmetric Jacobian requires that each flow element: (1) connect to exactly two zones; and (2) calculate the airflow as a function of the pressure difference between those zones. These requirements follow from the fact that the Jacobian expresses the derivatives of the mass flows with respect to the zone reference pressures. Symmetry implies that the flow through a path must not change if the reference pressures in the zones it connects both change by the same amount.

Another important design decision was to require positive-definite system matrices. This requirement was adopted because a system that always produces symmetric positive-definite Jacobians must have a unique solution (Lorenzetti, 2002). Furthermore, relatively simple search algorithms can always find that solution. Finally, a positive-definite matrix simplifies the factorization algorithm still further.

In practical terms, a positive-definite Jacobian requires that: (1) each flow element gives more positive flow with more positive pressure drops in the flow direction; and (2) each zone connects, directly or indirectly, to at least one zone of known pressure. Most real flow elements satisfy the first criterion (Lorenzetti, 2002). The second requirement relates to the building topology, rather than to the component models individually.

The restrictions described above ensure the airflow systems have desirable mathematical prop-

erties. In addition, CONTAM and COMIS simplify the flow element models for convenience of implementation. Specifically, when they calculate the mechanical energy "lost" in each flow path, they do so independently of the flow path calculations. This "lost" energy represents the conversion of mechanical to thermal energy by viscous dissipation. It is a primary component of the pressure drop that forces air through the flow path. However, that pressure drop also depends on changes of potential energy (due to changes of height) and kinetic energy (due to changes of the velocity profile of air) through the flow path (McQuiston and Parker, 1988).

By calculating this lost energy outside of the flow path model, the programs simplify the code. In particular, imposing a global assumption about the energy balance frees the flow models from having to solve the energy and pressure-flow relations simultaneously. Unfortunately, this simplification prevents the model developer from representing more complicated relationships between the zone pressures, the density and velocity profiles of air in the path, and the mass flow of air through the path.

Unsupported Models

The design decisions made in CONTAM and COMIS make it difficult to implement some models, and impossible to implement others. This section describes some potentially useful and important models that the programs do not currently support. It identifies which models do not meet the fundamental restrictions imposed by the programs, and which could be implemented within the current framework, given sufficient programming effort.

The fact that each zone must have a single state variable (its reference pressure) precludes any momentum-balancing zone model. Thus no formulation based on the Navier-Stokes equations, such as the SIMPLE algorithm (Patankar, 1980), may be used to predict flow details within rooms. Note that it is possible to predict intra-room flows using the subzonal models described by Wurtz et al. (1999), because these rely on temperature correlations and standard multizone flow elements, and do not introduce any new state variables to the airflow system.

Similarly, flow elements cannot incorporate momentum, since they must calculate steady-state flows based on the pressure difference between the zones they connect. Modeling momentum could be important in cases where a control system tries to quickly reduce the flow in a duct system, for example to shut off flow after detecting a pollutant in the supply air. In a real system, flow through a closing damper could be much greater than a steady-state model would suggest. Fortunately, in most applications a quasi-steady simulation, which approximates the dynamics by running a fan or damper model through a series of steady states, probably suffices.

Another dynamic of interest in duct systems, and one of potentially greater significance, concerns the delays associated with pollutant transport in flow paths. CONTAM and COMIS do not directly model transport delays, which would require them to account for both the pollutant mass stored in the flow paths, and the time needed to carry it between zones. Modeling all transport as instantaneous simplifies the assembly of the defining equations, but over-predicts the speed at which pollutants spread through a building. Fortunately the user may force the program to account for transport delays, by breaking up a flow path into a number of subpaths, connected in series between zones of appropriate volume. However this technique is less than ideal, as it complicates the model's input requirements, and unnecessarily increases the number of equations in the airflow system.

Restricting flow elements to depend on the pressure drop between two zones precludes proper modeling of duct T-junctions. Junctions, as three-port flow elements, cannot be defined solely in terms of pressure differences, because the mechanical energy dissipated in each branch of a junction depends on the flows in the other branches (McQuiston and Parker, 1988). Hence, they destroy symmetry in the system Jacobian. Modeling T-junctions properly would be very costly, in both storage and factorization times for the system matrices. Unfortunately, no simulation that demands fidelity in the duct system representation, for example as part of a duct design procedure, can ignore the pressure-flow characteristics of junctions. First, fitting losses usually exceed losses in a straight pipe. Second, junctions have unique characteristics among fittings. For example, changing the flow in one branch can even produce suction on another branch that previously faced a retarding pressure.

The fact that CONTAM and COMIS decouple the energy balance from the flow element relations

means they cannot properly model buoyancy-driven bidirectional flow across a horizontal partition. For small pressure differences across the gap, the flow model must solve for the dissipated energy and the flow simultaneously, but the program design prevents this. This becomes important in, for example, a stairwell or elevator shaft, where temperature differences between floors of a building can set up recirculation between floors (Edwards and Irwin, 1990). In cases of natural ventilation, or forced ventilation where the mechanical system design tends to isolate floors, the programs may not predict two-way flows between floors. Note however that they can accurately model unidirectional, mechanically-driven flows in stairways (Feustel et al., 1985).

Conclusion and Implications

Design decisions made in CONTAM and COMIS prevent them from implementing a number of potentially useful models. These include: (1) certain types of dynamic behavior; (2) detailed duct systems; (3) pollutants that do not satisfy the well-mixed assumption; and (4) mixed natural and forced convection across horizontal partitions.

Some of these limitations derive from fundamental structural issues, like the reliance on symmetry-preserving flow elements. Others result from implementation details that could be resolved within the existing framework of the programs, such as the decoupled energy balance relation.

For users who wish to apply these programs to certain types of problems, these limitations may increase the need to modify or replace the programs. In particular, those interested in novel ventilation control systems, duct system design, or natural or hybrid ventilation, will find the programs' limitations outweigh their strengths as environments for simulating whole-building airflow and pollutant transport.

An effort should be made to identify and test alternate simulation environments. Desirable features include: (1) the ability to mix algebraic and differential equations when defining component models; (2) event-based models, for example to simulate a control system whose mode changes based on data from a pollutant sensor; (3) general nonlinear equation solvers, including a variety of direct and indirect matrix techniques; (4) an intuitive user interface for connecting component models in order to build up systems; and (5) support for wholly modular components, that is, an architecture that keeps the code for component models separate from the code that performs the simulation.

Acknowledgements

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